

REPORT DOCUMENTATION PAGE				Form Approved OMB No. 0704-0188	
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1. REPORT DATE (DD-MM-YYYY) 08-07-2010		2. REPORT TYPE Technical Paper		3. DATES COVERED (From - To)	
4. TITLE AND SUBTITLE  The Internal Flow Modeling of a Simulated Solid Propellant-Liner Debond Using Loci-CHEM				5a. CONTRACT NUMBER FA8650-09-M-2028	
				5b. GRANT NUMBER	
				5c. PROGRAM ELEMENT NUMBER	
6. AUTHOR(S) Caroline Hood & Joe Sims (Analytical Services, Inc.)				5d. PROJECT NUMBER	
				5e. TASK NUMBER	
				5f. WORK UNIT NUMBER 300509WY	
7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES)  Analytical Services, Inc. 350 Voyager Way Huntsville AL 35806				8. PERFORMING ORGANIZATION REPORT NUMBER  AFRL-RZ-ED-TP-2010-317	
9. SPONSORING / MONITORING AGENCY NAME(S) AND ADDRESS(ES)  Air Force Research Laboratory (AFMC) AFRL/RZS 5 Pollux Drive Edwards AFB CA 93524-7048				10. SPONSOR/MONITOR'S ACRONYM(S)	
				11. SPONSOR/MONITOR'S NUMBER(S) AFRL-RZ-ED-TP-2010-317	
12. DISTRIBUTION / AVAILABILITY STATEMENT  Approved for public release; distribution unlimited (PA #10324).					
13. SUPPLEMENTARY NOTES For presentation at the 46 <sup>th</sup> AIAA/SME/SAE/ASEE Joint Propulsion Conference, Nashville, TN, 25-28 July 2010.					
14. ABSTRACT To determine whether a flawed solid propellant would be safe for operational use, one must first verify whether the flaw, which can take form as a crack or fracture (a volume between two propellant surfaces) or a debond (a volume between propellant and liner), will propagate or simply burn out after it ignites. A prediction of whether the flaw will propagate, and to what extent it will propagate, can be made by calculating the pressure distribution inside the burning flaw and then the resultant stress/strain field generated in the solid propellant. However, to precisely predict the pressure distribution and stress/strain field, the flow field, especially at the crack tip, has to be thoroughly understood. The work described herein mainly focused on studying the gas dynamic behavior inside a simulated solid propellant flaw using a computational fluid dynamics approach. In this effort, a finite-volume, density-based Navier-Stokes solver called Loci-CHEM was used. The code replicated experimental results with reasonable accuracy and showed little sensitivity to grid resolution and gas properties assumptions. The pressure distribution was affected by the assumed level of turbulence intensity, which has led to the development of a linearized flow instability model that may be used in the future to better predict turbulence inside burning flaws. Future efforts will use fully coupled fluid dynamics and structural dynamics codes to more accurately predict flaw propagation.					
15. SUBJECT TERMS					
16. SECURITY CLASSIFICATION OF:			17. LIMITATION OF ABSTRACT	18. NUMBER OF PAGES	19a. NAME OF RESPONSIBLE PERSON
a. REPORT	b. ABSTRACT	c. THIS PAGE			Lt. Nathaniel Knight
Unclassified	Unclassified	Unclassified	SAR	8	19b. TELEPHONE NUMBER (include area code) N/A

# The Internal Flow Modeling of a Simulated Solid Propellant-Liner Debond Using Loci-CHEM

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To determine whether a flawed solid propellant would be safe for operational use, one must first verify whether the flaw, which can take form as a crack or fracture (a volume between two propellant surfaces) or a debond (a volume between propellant and liner), will propagate or simply burn out after it ignites. A prediction of whether the flaw will propagate, and to what extent it will propagate, can be made by calculating the pressure distribution inside the burning flaw and then the resultant stress/strain field generated in the solid propellant. However, to precisely predict the pressure distribution and stress/strain field, the flow field, especially at the crack tip, has to be thoroughly understood. The work described herein mainly focused on studying the gas dynamic behavior inside a simulated solid propellant flaw using a computational fluid dynamics approach. In this effort, a finite-volume, density-based Navier-Stokes solver called Loci-CHEM was used. The code replicated experimental results with reasonable accuracy and showed little sensitivity to grid resolution and gas properties assumptions. The pressure distribution was affected by the assumed level of turbulence intensity, which has led to the development of a linearized flow instability model that may be used in the future to better predict turbulence inside burning flaws. Future efforts will use fully coupled fluid dynamics and structural dynamics codes to more accurately predict flaw propagation.

## Nomenclature

$A$	=	burn rate coefficient
$C_p$	=	constant pressure specific heat
$k$	=	turbulent kinetic energy
$n$	=	burn rate exponent
$p$	=	pressure
$\Delta s$	=	grid spacing
$\varepsilon$	=	turbulent dissipation
$\gamma$	=	ratio of specific heat
$\omega$	=	specific dissipation

## I. Introduction

Through time, a solid propellant goes through slowly-evolving chemical changes (e.g., diffusion of active chemical species, energetic material decomposition, etc.) that result in a reduction of mechanical properties. As they age, a substantial portion of the propellant grain can become either brittle or soft, depending upon its proximity to liners and insulators and upon the propellant's formulation. Additionally, cumulative damage can occur as the

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motor is subjected to rough handling loads, temperature cycling and slumping from gravitational accelerations. As a result, it is critically important to understand the actual state of aged propellant prior to its use in the field or on a test stand. The use of X-rays, computed tomography (CT) scans, and other non-destructive evaluation (NDE) methods is a routine part of many motor programs. Those evaluations do not measure propellant mechanical properties, but they can detect flaws (e.g., propellant cracks along the bore and in slots, bondline de-bonds, etc.) that pose a serious risk to a motor's integrity. To do that, propellant samples are often cut from aged motors so that mechanical properties can be measured directly. These tandem approaches have, for the most part, protected against failures of aged motors and allowed questionable assets to be removed from the inventory.

Whenever a flaw is detected in a motor, the fundamental question that decision makers must contend with is whether the detected flaw will propagate. The logical follow-on question to that one, assuming the flaw will propagate, is whether it will propagate to the motor's destruction. The answers to those questions are complex, incompletely understood, and usually little more than educated guesses.

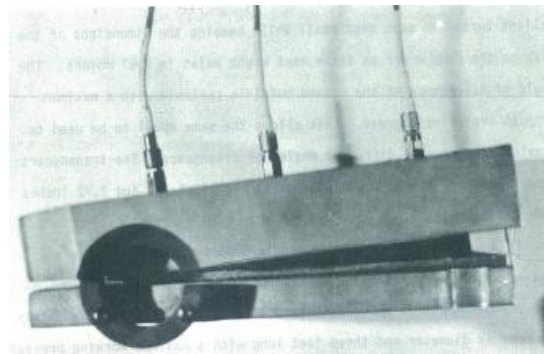
The reason that is so is because predicting flaw propagation in a propellant grain requires detailed understanding of at least three distinct engineering domains. For accurate prediction, one must understand the transient fluid dynamics and flame spreading behavior within the flaw volume; the resultant stress, strain and strain rate field that develops in the nonlinear viscoelastic propellant; and the fracture mechanics behavior at or near the crack tip region, which acts as a stress concentration riser. More importantly, for the highest accuracy prediction, each of these domains must be dealt with in a fully coupled manner.

The disciplines have reached a maturity level that can, with reasonable accuracy, numerically represent the majority of the physical phenomenon associated with it. Thus, the overall goal driving the efforts summarized here is to develop a fully-coupled multi-physics computational tool that used the best representative tool from each of the three domains. Such a tool would give decision makers more information on which to base their go/no-go decisions and would do so with a higher confidence factor. The first step in creating that tool was to verify that a modern CFD tool could accurately simulate the combustion and flow inside a burning flaw. Thus, the objective of this study was simply to demonstrate the feasibility of using the density-based, finite-volume, parallel Navier-Stokes solver called Loci-CHEM code to accurately simulate the fluid dynamic behavior inside a simulated propellant-liner debond. A comparison was made between the Loci-CHEM results and a set of experiments that was conducted in the early 1970's. This validation was crucial for determining the numerical requirements (grid resolution, sensitivities to assumptions, etc.) to achieve high accuracy.

## II. Description of the Experimental Data in the Literature

A comprehensive set of labscale experiments was carried out in the early 1970's in which the researchers developed an experimental apparatus to simulate the combustion gas flow inside a propellant-liner debond and measured the pressure distribution along the simulated flaw<sup>1</sup>.

The test article, reproduced from Ref. 1 in Figure 1, was an adjustable wedge that had a propellant slab on its lower half and three pressure transducers installed on its upper half. Two 0.25" thick plexiglas side pieces were used to enable photographic visualization of burning processes. The propellant slab was 0.1" thick (measured prior to ignition) and the dimensions of its burning surface were 3" wide and 4.5" long. The pressure transducers were placed at 0.19, 1.72 and 3.72" from the debond tip. In order to simulate the externally imposed chamber pressure that exists in a rocket motor, the entire apparatus was placed inside a chamber that included pressure control devices such that the flow Mach number inside the simulated flaw could be controlled by simply varying the wedge angle. Both nitrogen and air with a range of simulated pressure were used to pressurize the chamber. The debond angles and corresponding chamber pressures used by the researchers are summarized in Table 1.



**Figure 1. Debond test article used in Ref. 1**

To complement that experimental study, Jacobs, et. al. also conducted a one-dimensional steady-state analysis of a burning flaw using a closed-form analytical method. A comparison was made between the numerical solutions and the experimental results. The detailed explanations of the analytical method used can be found in Ref. 1.

One discrepancy concerns the propellant used in [1]. The authors reported using an aluminized double base (DB) propellant that was described as (then) Thiokol's TP-H1011 formulation. However, the Chemical Propulsion Information Agency's (CPIA) solid propellant database entry<sup>2</sup> for TP-H-1011 shows that it is an aluminized AP (ammonium perchlorate) composite propellant. Beyond the differences in propellant composition and resultant combustion gas properties, there was a substantial difference in burn rates reported in Ref. 1 and Ref. 2, which obviously result in differences between the CFD predicted pressure distribution, the experimental data, and the closed-form analytical solution shown in Ref. 1. Ultimately, the gas properties and burn rate variables reported in Ref. 1 were used in the present study to allow direct comparison between CFD results, the closed-form analytical solutions, and the experimental data.

Wedge Angle	Pressures (psi)	Flow Regime
4.75°	170, 300, 400	Subsonic
3.17°	332	Subsonic
1.9°	550, 600	Subsonic
0°	245	Sonic

**Table 1. Experimental set points.**

### III. Computational Tool: Loci-CHEM

CHEM is a density-based, finite-volume, parallel Navier-Stokes solver for generalized grids using the Loci framework developed at Mississippi State University in part through NASA and NSF funded efforts<sup>3</sup>. Because it can use either structured or unstructured grids, Loci-CHEM is convenient for complex geometries. It is second-order accurate in both space and time, and uses high resolution approximate Riemann solvers to solve turbulent flows. CHEM can solve chemically reacting flows, from simple equilibrium to complex multi-species, multiple-reaction finite rate chemistry models. Several kinetics models are already built-in, and have been used to model the internal flow of LOX-hydrogen propellant rockets<sup>4</sup>. However, its capability for modeling the combustion and internal flow of solid rocket motors is still under development. There are three main features of modeling solid propellant combustion absent from the basic distribution of Loci-CHEM.

First, a boundary condition that models the mass addition from the burning surface is not available in the basic distribution of Loci-CHEM. However, an extension module was developed by Tetra Research Corporation that adds a pressure dependent mass flux boundary condition based on the  $Ap^n$  theory<sup>5</sup>. This module was used in this study.

Second, the program does not support moving boundaries and/or meshes that are needed to account for the propellant surface regression. Another module that will add the capability is currently being developed, but was not ready for use in this effort. Instead, a quasi-steady state assumption was used where the propellant surface was assumed to be ignited everywhere instantaneously. Commonly used in standard internal ballistics calculations, the quasi-steady assumption was reasonable given that the summary data in Ref. 1 were taken shortly after ignition. Detailed photographic studies assured those researchers that the entire propellant surface was ignited quickly. Also, a special high burn rate coating was applied to each propellant sample to insure rapid ignition.

Lastly, Loci-CHEM does not support multi-phase flow, when in fact some of the solid particles released from the surface do not burn instantaneously. Thus, in the strictest sense, the flow cannot be treated as purely Eulerian. However, it is believed that non-Eulerian effects to the overall pressure distribution inside the debond simulator are negligible.

## IV. Results

### A. Model Implementation

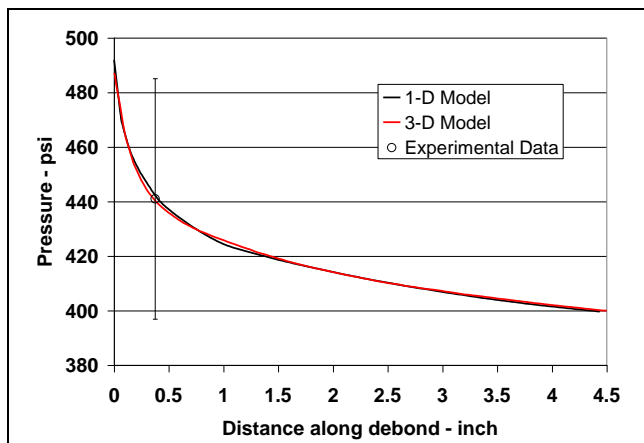
Menter's Shear Stress Transport (SST) model built on a baseline model, namely the baseline (BSL) model<sup>6</sup>, was used in the current effort. The model combines the Wilcox  $k-\omega$  model in the near-wall region with the  $k-\epsilon$  model in the outer part of the boundary layer. An assumption of equilibrium chemistry and constant viscosity were used to

model the combustion gas. The three-dimensional mesh was generated using GRIDGEN Version 15. An anisotropic mesh was generated by extrusion to accurately represent the boundary layer along solid surfaces. The remainder of the computational domain was meshed using unstructured cells.

As mentioned previously, the burning propellant surface boundary condition was used, along with impermeable wall boundaries to represent solid walls. The downstream exit boundary condition was an outflow with an imposed back pressure. The computational domain was initialized with a given pressure and temperature to start the steady state simulation. The model was executed in local time stepping mode with a physical time step of 0.01 seconds. This time step was dynamically reduced by the Loci-CHEM solver in the event that a local Courant–Friedrichs–Lewy (CFL) number exceeded 5,000 or a change in temperature, pressure or density of more than 5 percent occurred in one time step. Using these settings, the simulation required about 2,000 time steps to converge to a steady state solution. Convergence was evaluated by observing the drop in residuals and by observing volume probes of temperature and pressure at several locations throughout the flowfield.

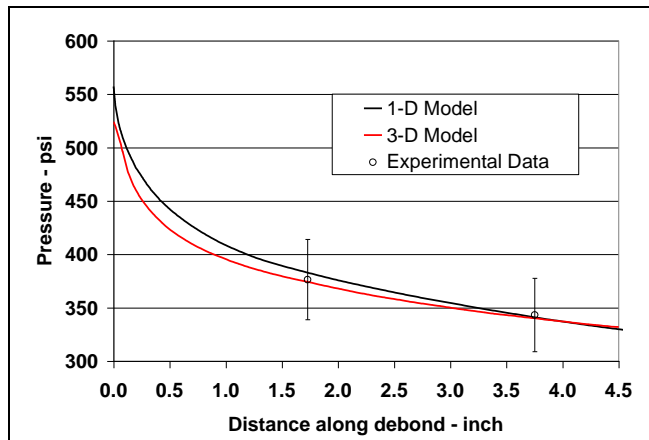
## B. Baseline Results

Figure 2 shows a comparison between the Loci-CHEM solution, the baseline 1-D solution (Jacobs' 1-D analytical model<sup>1</sup>), and the experimental measurement<sup>1</sup> along with 10 percent error bars for debond angle and pressure chamber of  $4.75^\circ$  and 400 psi respectively. The results show excellent agreement among all three results. The 1-D model and 3-D CFD results are virtually identical and both profiles pass neatly through the measurement error bars (downstream measurement results were not available for comparison). There is a small deviation between the fluid dynamic models near the crack tip, as the 1-D model predicts a debond tip pressure of about 500 psi, whereas the 3-D CFD solution predicts about 485 psi at the tip (~2.5% difference, which is likely within the uncertainty of both the CFD solution and 1-D model). Experimental data were not collected at the debond tip, so it is not apparent which solution is correct. Similar pressure profile agreement is also observed for the same debond



**Figure 2. Comparison between analyses and experiment at  $4.75^\circ$  and 400 psi.**

angle with chamber pressures of 300 and 170 psi.



**Figure 3. Comparison between analyses and experiment at  $3.17^\circ$  and 330 psi.**

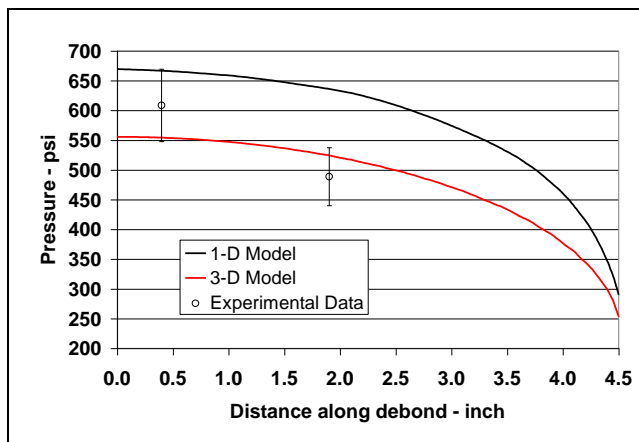
a difference of ~18% in pressure at the debond tip.

Figure 3 shows the results comparison for a smaller debond angle and lower chamber pressure. For this analysis, the debond angle was reduced to  $3.17^\circ$  and the chamber pressure was set to about 332 psi. There is slightly a higher difference of the results of the pressure calculation at the debond tip of ~6%, which might be caused by a higher Mach number flow inside the debond due to a smaller volume. However, an overall good agreement was obtained for this analysis.

One particular experiment was purposely designed to induce choked flow within the debonded volume and, as a result, the fluid dynamics changed significantly. Figure 4 shows the comparisons. In this instance, the CFD solution appears to be better, compared to the experimental data, than the 1-D solution. There is

There were several important conclusions to this baseline set of analyses. First, the CFD represented the general physics of the particular problem faithfully: the difference in bulk flowfield behavior between low subsonic flow (high wedge angle, low chamber pressure) and sonic flow ( $0^\circ$  wedge angle, high chamber pressure) is clearly captured by the CFD model with no special additional input required. Second, despite some small quantitative differences between experimental measurements and CFD results, the correspondence between the two is qualitatively excellent. To better understand those quantitative differences, a subset of analyses was completed that highlighted the sensitivity of the CFD results to several assumptions.

As discussed previously, the flowfield inside the simulated flaw is sensitive to the actual size of the crack tip gap and to the overall empty volume, both of which constantly changed throughout a test due to the propellant regression. Unfortunately, the researchers did not record in Ref. 1 exactly when any particular pressure measurement was made in any given test. They merely stated that each dataset came from within the first 0.1 to 0.5 seconds of any given test. This made it impossible to determine whether the idealized numerical domain, shown in the figure below, truly represented the flaw tip gap and overall empty volume for any of the experimental results. In every case, the numerical domain used pre-test dimensions of the hardware and propellant slab.

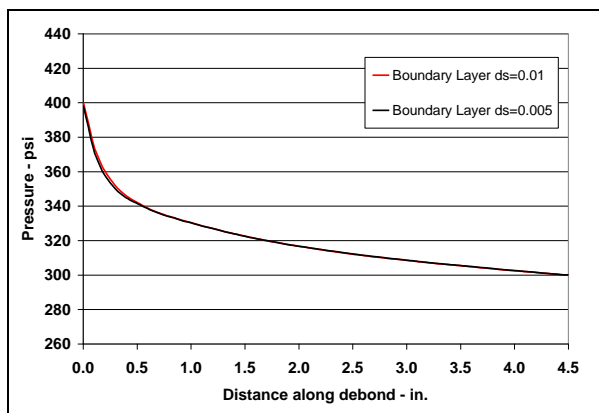


**Figure 4. Comparison between analyses and experiment at  $0^\circ$  and 245 psi.**

However, it was also important to understand better how several assumptions affected the CFD results, since future analyses on real motor flaws will have analysts grapple with much of the same geometric uncertainty. In fact, they will likely face uncertainties in flaw geometry to a far greater extent, since NDE equipment generally do not have high resolution.

Therefore, several sensitivity analyses were completed. First, a grid sensitivity study was performed to understand whether grid independence had been achieved. This was followed with an analysis to determine how sensitive the results were to assumptions of gas properties. Finally, the effect of turbulence level assumptions was analyzed. All of these results are shown in the following sections.

### C. Grid Sensitivity Study



**Figure 5. Grid resolution study results.**

Figure 5 shows a comparison between two different grid densities; the  $\Delta s$  term is the factor that controls grid spacing. In this instance, the spacing factors of 0.01 and 0.005 are used (i.e., the second grid used spacing half as much as the first), which roughly translates into a mesh density increase by a factor of eight, via a doubling of the number of grid points along all three primary dimensions. The results between the two analyses are nearly identical, showing that a grid independent solution was obtained.

### D. Combustion Gas Properties Sensitivity Study

Even with very complex solid propellant simulations addressing other difficult problems facing solid rocket motors, complex chemical kinetic models are not often necessary<sup>7</sup>. It was assumed that such will

be the case for the flaw propagation problem, since gross flowfield properties of pressure and Mach number are only moderately affected by chemical non-equilibrium (local temperature is, of course, the primary affected property). Thus the baseline results reported here reflect the assumption of chemical equilibrium. Properties were generated

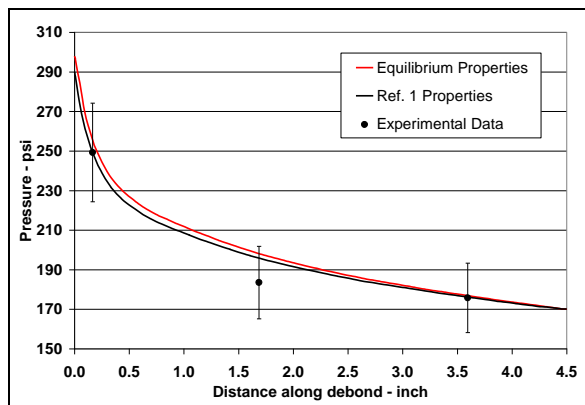
using the NASA CEA2 code, the current version of the venerable code developed by Gordon and McBride starting in the early 1960's. CEA2 was used to calculate specific heat ( $C_p$ ), ratio of specific heats ( $\gamma$ ), adiabatic flame temperature and density. Recall also that there was considerable uncertainty in the actual propellant tested in Ref. 1.

To better understand how sensitive the baseline results were, an additional analysis was completed that used the (frozen) combustion gas properties reported in Ref 1. Figure 6 shows that it does make a small difference to the CFD results, especially near the flaw tip region, but all results fell within the estimated uncertainty of the measurements. For the baseline analysis, it appears that equilibrium assumptions are satisfactory.

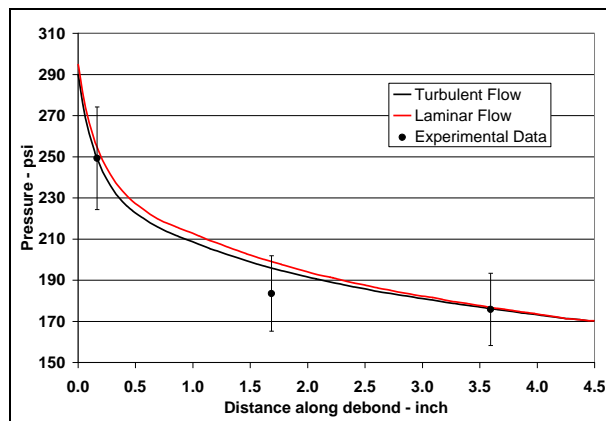
### E. Turbulence Level Sensitivity Study

After an extensive review, the literature does not show a discernible trend regarding turbulence assumptions for burning flaw flowfield simulation. In fact, the review shows a roughly even division between simulations that assumed laminar flow and ones that assumed turbulent flow. Given that solid rocket propulsion typically exhibits highly turbulent flow within the grain perforation, it seems natural to assume that the flow within a flaw would likewise be turbulent. However, it also seems reasonable to assume that the flow will transition from laminar to turbulent, similar to any non-combusting channel or pipe flow.

To understand the sensitivity of the CFD results to turbulence assumptions, an analysis was completed using a fully laminar assumption. The results, shown in Figure 7, show a higher pressure near the crack tip, due to lower irreversible losses; as with the other sensitivity analyses, the difference seen is well within the experimental uncertainty. The best understanding at the moment is that the flow inside a burning flaw will probably transition from laminar to turbulent.



**Figure 6. Combustion gas properties sensitivity study results.**



**Figure 7. Turbulence intensity sensitivity study results.**

## V. Conclusions

The goal of the current study was to demonstrate feasibility of using a modern CFD tool to predict the flowfield inside a solid propellant grain's burning flaw. This is the first step to realizing the use of a multiphysics approach to simulate flawed solid rocket. The baseline analyses, along with the understanding of the drivers behind the minor discrepancies shown between the CFD results and the experimental results, clearly demonstrate feasibility of such approach. Sensitivity analyses showed that assumptions regarding grid resolution, chemical non-equilibrium, and turbulence level are relatively modest for such a simple geometry. Actual flaws are not expected to show low sensitivity. Realistically, specification of turbulence levels likely provide the largest source of sensitivity, so work remains in understanding the stability of the flow inside a burning flaw. Prediction of crack tip pressure is affected by the level of turbulence, so assumptions must be accurate in order to increase the accuracy of future flaw propagation predictions.



## Acknowledgments

The support from the U.S. Air Force under SBIR contract number FA8650-09-M-2028 is gratefully acknowledged.

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